

Single Photon Position and Momentum Uncertainty Relations

G. Guarnieri, M. Motta and L. Lanz

Dipartimento di Fisica, Università degli Studi di Milano, via Celoria 16, 20133 Milano, Italy

(Dated: March 26, 2014)

We provide a single photon formalism where the suppression of 0-helicity photon states is identified, by only means of the conditions of spin $s = 1$ and mass $m = 0$, as a projection from an ancillary Hilbert space onto the physical Hilbert space, which carries an irreducible representation of the Poincaré group, leading immediately to momentum and polarization observables. By virtue of this new framework it becomes moreover possible to introduce in a natural way the single-photon position and spin as Positive Operator Valued Measures (POVMs), obtained through the application of the projection from usual self-adjoint operators on the ancillary Hilbert space. Finally Heisenberg uncertainty relations for position and momentum are extensively studied, and the effect of the projection operator is quantified by exploring single photon gaussian states, for several choices of spin and polarization.

PACS numbers: 03.65.Ca, 14.70.Bh, 03.65.Ta

I. INTRODUCTION

The investigation of single photon properties has experienced an increasing interest in the last years¹⁻⁴. The reason has to be sought in the escalating request, in many quantum information and cryptography protocols⁵, for highly accurate manipulations of spatial and polarization single-photon properties.

The aim of the present work is to delineate a single photon formalism which allows to introduce and study the usual fundamental observables (e.g. spin, position, momentum) in the context of the modern axiomatics of quantum mechanics as Positive Operator Valued Measures (POVMs), this way reconsidering and generalizing the treatment of the photon position given by Kraus⁶. This construction represents a new perspective which allows to face, in a very natural way, the notoriously delicate problem of photon localization^{7-10,12-14}. By making use of an irreducible unitary representation of the Poincaré group for spin 1 and mass 0 particles, consistent with the seminal work by Wigner¹¹, we show that the suppression of the 0-helicity states can be interpreted as the action of a projection operator from an auxiliary Hilbert space to the physical Hilbert space. This projection naturally brings along the notion of POVMs, obtained from Projection-Valued Measures (PVMs) of observables associated to self-adjoint operators in a wider Hilbert space (a mechanism known as Naimark's Theorem¹⁵). In particular we consider position, momentum and spin observables and discuss the consequent Heisenberg uncertainty relations. The effects of such projection on gaussian states, which in non-relativistic framework saturate the inequality $\Delta X_k \Delta P_k = \frac{\hbar}{2}$, is studied. In Section II a description of the underlying formalism is given (see Supplemental Material for further details). In Section III, observables are defined, following the typical construction of open quantum systems theory, in terms of POVMs. In the two following Sections, detailed results relative to gaussian states are presented, and conclusions are given in Section V.

II. SINGLE-PHOTON STATES

The quantum mechanical description of a *non-relativistic* particle with spin $s = 1$ takes place in the Hilbert space $\mathcal{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^3$ with inner product $\langle \phi | \psi \rangle = \sum_{j=1}^3 \int d^3p \phi_j^*(\mathbf{p}) \psi_j(\mathbf{p})$, on which the familiar¹⁶ unitary representation of the roto-translation group can be defined as follows:

$$(\psi')^j(\mathbf{p}) = e^{-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{a}} \sum_{k=1}^3 \left(e^{-\frac{i}{\hbar} \phi \mathbf{n} \cdot \mathbf{S}} \right)_k^j (\psi)^k(R^{-1}\mathbf{p}) \quad (1)$$

where R is the matrix associated to the rotation of an angle φ around the axis \mathbf{n} and \mathbf{S} denotes the Pauli vector of spin matrices

$$s_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} s_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & i & 0 \\ -i & 0 & i \\ 0 & -i & 0 \end{pmatrix} s_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (2)$$

R and \mathbf{S} are related to each other by¹⁷

$$R = V^\dagger e^{-\frac{i}{\hbar} \varphi \mathbf{n} \cdot \mathbf{S}} V \quad (3)$$

where the unitary matrix V reads¹⁸

$$V = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & -1 \\ -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \end{pmatrix} \quad (4)$$

The key relation (3) is a peculiar prerogative of the spin $s = 1$ case.

The photon anyway is a purely relativistic object and thus the description given above does not suit the purpose. In order to accomplish this task, we can exploit relation (3) to notice that the wavefunction $V^\dagger \psi(\mathbf{p}) \equiv \psi_V(\mathbf{p})$ transforms as a vector field

$$(\psi'_V)^j(\mathbf{p}) = e^{-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{a}} \sum_{k=1}^3 R_k^j (\psi_V)^k(R^{-1}\mathbf{p}) \quad (5)$$

It becomes natural to generalize the formalism outlined above by means of the following procedure:

- endowing the wavefunction with a fourth component, $\psi_V^0(p)$, this way promoting it to a four-vector which transforms under the Poincaré group (a, Λ) as

$$(\psi'_V)^\mu(p) = e^{\frac{i}{\hbar} a_\tau p^\tau} \Lambda^\mu_\nu \psi_V^\nu(\Lambda^{-1}p) \quad (6)$$

which is a direct generalization of (5).

- equipping the space of the four-vectors $\mathcal{H} = \mathcal{L}^2\left(\mathbb{R}^3, \frac{d^3p}{p^0}\right) \otimes \mathbb{C}^4$ with the following sesquilinear form

$$\langle \phi_V | \psi_V \rangle = - \int \frac{d^3p}{p^0} (\phi_V^\mu)^*(p) g_{\mu\nu} \psi_V^\nu(p) \quad (7)$$

which reduces to the usual scalar product when $\psi_V^0(p) = 0$ and for which the transformation $U(a, \Lambda)$ is an isomorphism. We notice that the Poincaré invariant measure $\frac{d^3p}{p^0}$ replaces the non-relativistic roto-translationally invariant Lebesgue measure d^3p .

The non-positivity of the scalar product (7) in the *pseudo-Hilbert space* \mathcal{H} ,¹⁹ which is the direct consequence of the non-positive Minkowski inner product, prevents from giving a probabilistic interpretation to the theory. Nevertheless, this fact can be overcome in the special case of massless particles such as photons. In fact, as exposed in more detail in the Supplemental Material, the massless condition naturally identifies a subspace $\mathcal{S} \subset \mathcal{H}$

$$\mathcal{S} = \{|\psi_V(p)\rangle : p^\mu g_{\mu\nu} \psi_V^\nu(p) = 0 \text{ for almost all } p\} \quad (8)$$

where the restriction of (7) results to be non-negative.

To see this fact, let us introduce the *intrinsic frame* $\{\tilde{e}_\mu(\mathbf{p})\}_{\mu=0,\dots,3}$, obtained by rotating the canonical lorentzian basis so that $\tilde{e}_3(p) = (0, \frac{\mathbf{p}}{|\mathbf{p}|})$; equation (8) can then be recast in the more intelligible form

$$\mathcal{S} = \{|\tilde{\psi}(p)\rangle : p^0 \tilde{\psi}_V^0(\mathbf{p}) - |\mathbf{p}| \tilde{\psi}_V^3(\mathbf{p}) = 0\} \quad (9)$$

$$\xrightarrow{p^\mu p_\mu = 0} \{|\tilde{\psi}_V(p)\rangle : \tilde{\psi}_V^0(\mathbf{p}) = \tilde{\psi}_V^3(\mathbf{p}) \quad \forall \mathbf{p} \in \mathbb{R}^3\}$$

(where in the last equivalence we explicitly used the massless condition). The restriction of the scalar product (7) to this subspace reads

$$\langle \phi_V | \psi_V \rangle = \int \frac{d^3p}{p^0} \left((\tilde{\phi}_V^1)^*(p) \tilde{\psi}_V^1(p) + (\tilde{\phi}_V^2)^*(p) \tilde{\psi}_V^2(p) \right) \quad (10)$$

Equation (10) indicates that the component $\tilde{\psi}_V^3(p) = \tilde{\psi}_V^0(p)$ is a redundant degree of freedom, being precursory of the *gauge* symmetry in electromagnetism by basic aspects of quantum theory of a massless particle.

The pairs $(\tilde{\psi}_V^1(p), \tilde{\psi}_V^2(p))$ constitute the proper Hilbert space $\mathcal{H}_\mathcal{S}$ of a single photon, with inner product defined by (10). Relevant elements of this space are photon states with linear and circular polarization, which are respectively given by $(\alpha \tilde{\psi}_V(p), \beta \tilde{\psi}_V(p))$, $\alpha, \beta \in \mathbb{R}$ and $(\frac{\tilde{\psi}_V(p)}{\sqrt{2}}, \frac{\pm i \tilde{\psi}_V(p)}{\sqrt{2}})$.

It is moreover important to stress that the subspace $\mathcal{H}_\mathcal{S}$ carries an irreducible representation of the Poincaré group:

$$(\tilde{\psi}'_V)^i(p) = e^{\frac{i}{\hbar} a_\tau p^\tau} \sum_{j=1}^2 \tilde{e}_i^\mu(p) \Lambda_{\mu\nu} \tilde{e}_j^\nu(\Lambda^{-1}p) (\tilde{\psi}_V)^j(\Lambda^{-1}p) \quad (11)$$

in which the redundant component $\tilde{\psi}_V^3(p)$ is not involved. This construction has lead in a very natural way to the introduction of $\mathcal{H}_\mathcal{S}$ of single photons by just considering the conditions of zero mass and spin $s = 1$.

$\mathcal{H}_\mathcal{S}$ appears to be a subspace of an auxiliary Hilbert space $\mathcal{H}_\mathcal{A} = \mathcal{L}^2(\mathbb{R}^3, \frac{d^3p}{p^0}) \otimes \mathbb{C}^3$ of elements of the form

$$f_V(p) = \sum_{i=1}^3 \tilde{\psi}_V^i(p) \tilde{e}_i(p) \quad \left(\tilde{\psi}_V^1(p), \tilde{\psi}_V^2(p) \right) \in \mathcal{H}_\mathcal{S} \quad (12)$$

obtained by means of the projection operator

$$\pi : \mathcal{H}_\mathcal{A} \rightarrow \mathcal{H}_\mathcal{S}, \quad \pi_k^j(p) = \delta_k^j - \frac{p^j p_k}{|\mathbf{p}|^2} \quad (13)$$

which eliminates the longitudinal component of the triple $f_V^i(p)$ $i = 1, 2, 3$, retrieving Kraus' results¹⁴.

Moreover, by making an alternative choice for the ancillary Hilbert space, namely $\overline{\mathcal{H}}_\mathcal{A} = V \mathcal{H}_\mathcal{A}$, it becomes evident that the physical subspace $\mathcal{H}_\mathcal{S}$, obtained now by means of the projection $V \pi V^\dagger$, corresponds to the subspace with non-zero helicity²¹. Finally, it is worth noticing that the transformation law (11), in the case of roto-translations, induces transformation (1) on $f^i(p) \in \overline{\mathcal{H}}_\mathcal{A}$, now in a relativistic context. Therefore the covariant observables of the non-relativistic theory become candidates for the relativistic scenery.

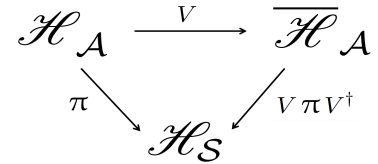


Figure 1. Diagram illustrating the action of the isomorphism V and projection π . Physical states are represented by couples $(\tilde{\psi}_V^1(p), \tilde{\psi}_V^2(p))$ in $\mathcal{H}_\mathcal{S}$. $|f_V\rangle$ in $\mathcal{H}_\mathcal{A}$ transform according to (5), while states $|f\rangle$ in $\overline{\mathcal{H}}_\mathcal{A}$ which transform with (1)

III. SINGLE PHOTON OBSERVABLES

The theory outlined above, and in particular the projection (13), has a prominent impact on single-photon observables. The embedding of \mathcal{H}_S in $\overline{\mathcal{H}}_A$ allows to define fundamental single-photon observables \hat{O} as self-adjoint operators on \mathcal{H}_A , even if \mathcal{H}_S is not closed under their action, due to the fact that $[\hat{O}, V\pi V^\dagger] \neq 0$.

In fact from the PVM $\hat{E}_O(M)$ associated to \hat{O} on $\overline{\mathcal{H}}_A$ one obtains the corresponding POVM $\hat{F}_O(\mathcal{M})$ on \mathcal{H}_S through the following general procedure:

$$\hat{F}_O(\mathcal{M}) = (V\pi V^\dagger) \hat{E}_O(\mathcal{M}) (V\pi V^\dagger) \quad (14)$$

For example, we have that momentum and spin operators admit the following representation on $\overline{\mathcal{H}}_A$:

$$\begin{aligned} (\hat{\mathbf{P}}f)_j(p) &= \mathbf{p} f_j(p) \\ (\hat{\mathbf{S}}f)_j(p) &= \sum_k \mathbf{S}_{jk} f_k(p) \end{aligned} \quad (15)$$

and their joint probability distribution in \mathcal{H}_S is then given by:

$$p(\mathbf{p} \in \mathcal{M}, S_z = s) = \int_{\mathcal{M}} d^3p \frac{1}{|\mathbf{p}|} \left| \sum_{i=1}^2 \tilde{\psi}_V^i(\mathbf{p}) [V\tilde{e}_i(\mathbf{p})]_s \right|^2 \quad (16)$$

In addition, motivated by previous work of Kraus⁶, we propose to introduce the photon position operator by generalizing the approach used in the relativistic description of massive particles, where localization experiments are given in terms of the Newton-Wigner operator²⁰:

$$(\hat{\mathbf{X}}f)_j(p) = i\hbar \frac{\partial f_j(p)}{\partial \mathbf{p}} - \frac{i\hbar}{2} \frac{\mathbf{p}}{(p^0)^2} f_j(p) \quad (17)$$

The definitions (14) and (17) yield the following joint probability distribution for position and spin:

$$p(\mathbf{X} \in \mathcal{M}, S_z = s) = \int_{\mathcal{M}} d^3x \left| \left[\tilde{\psi}_V(\mathbf{x}) \right]_s \right|^2 \quad (18)$$

in which the probability amplitude $\psi_s(\mathbf{x})$ reads:

$$\left[\tilde{\psi}_V(\mathbf{x}) \right]_s = \int \frac{d^3p}{|\mathbf{p}|} \sqrt{|\mathbf{p}|} \frac{e^{\frac{i}{\hbar} \mathbf{x} \cdot \mathbf{p}}}{(2\pi\hbar)^{\frac{3}{2}}} \sum_{i=1}^2 \tilde{\psi}_V^i(\mathbf{p}) [V\tilde{e}_i(\mathbf{p})]_s \quad (19)$$

It can be noticed that, by virtue of (5), this amplitude is covariant under roto-translations:

$$\tilde{\psi}'_V(\mathbf{x}) = e^{-\frac{i}{\hbar} \varphi \mathbf{n} \cdot \mathbf{S}} \tilde{\psi}_V(R^{-1}(\mathbf{x} - \mathbf{a})) \quad (20)$$

reproducing the expected transformation laws for the probabilities of spin and position. Moreover, the operators $\hat{\mathbf{X}}, \hat{\mathbf{P}}, \hat{\mathbf{S}}$ are irreducibly represented in $\overline{\mathcal{H}}_A$.

Expectation values and variances are immediately calculated from the probability distributions, obtained by means of (14).

A. Uncertainty Relations for Position and Momentum

In light of (18) and (16), it becomes interesting to investigate the Heisenberg uncertainty relations for position and momentum observables of a single photon. On $\overline{\mathcal{H}}_A$, where both these observables are defined in terms of self-adjoint operators with usual commutator $[X_{NW\ i}, P_j] = i\hbar \delta_{ij}$, the familiar inequality:

$$\Delta X_k \Delta P_k \geq \frac{\hbar}{2} \quad (21)$$

holds, and is saturated by gaussian states with definite spin along an arbitrary spatial direction. Equation (21) retains its validity on the physical space \mathcal{H}_S , but, due to π , it is no longer saturated by the minimum uncertainty states on $\overline{\mathcal{H}}_A$. In the following section, we will quantify the increase in $\Delta X_k \Delta P_k$ through an extensive study on both gaussian states with definite polarization and on projections of gaussian states with definite spin.

IV. RESULTS FOR GAUSSIAN STATES

A. States with Definite Polarization

We begin by studying in a detailed way the uncertainty relation for position and momentum of a photon considering gaussian states with definite polarization in \mathcal{H}_S :

$$\tilde{\psi}_V^i(\mathbf{p}) = \sqrt{|\mathbf{p}|} \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{8ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{4}}} e^{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{x}_0} \gamma^i, \quad \sum_{i=1}^2 |\gamma^i|^2 = 1 \quad (22)$$

being $\mathbf{p}_0 = \langle \hat{\mathbf{P}} \rangle$, $\mathbf{x}_0 = \langle \hat{\mathbf{X}} \rangle$ and, finally,

$$a = \frac{(\Delta p)^2}{2p_0^2} \quad (23)$$

a positive, dimensionless parameter which takes into account of the wavefunction's spread in momentum space.

Without any loss of generality, let us choose $\mathbf{p}_0 = |\mathbf{p}_0|e_z$. Applying the formalism detailed above and performing the calculations outlined in the Supplemental Material, we obtain the quantities $\Delta X_i \Delta P_i$, shown in figure 2. They are monotonically increasing functions of a . Remarkably, in the limit $a \rightarrow 0$, the minimum value $\Delta X_i \Delta P_i = \frac{\hbar}{2}$ is obtained, while in the limit $a \rightarrow \infty$, different asymptotic values are approached, given explicitly in the Supplemental Material.

B. Spin States

We now consider gaussian states with definite spin, defined on $\overline{\mathcal{H}}_A$:

$$[\mathbf{f}(\mathbf{p})]_i = \sqrt{|\mathbf{p}|} \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{8ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{4}}} \mathbf{e}_i \quad (24)$$

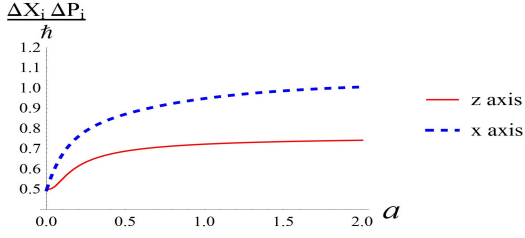


Figure 2. (color online): Heisenberg uncertainty products $\Delta x_i \Delta p_i$ in units of \hbar , along directions parallel (red solid line) and perpendicular (blue dashed line) to \mathbf{p}_0 , for states with definite polarization.

\mathbf{e}_i being the eigenstates of S_z .

The corresponding physical states are defined on \mathcal{H}_S as $[\tilde{\psi}_V(\mathbf{p})]_i = K [V\pi V^\dagger \mathbf{f}(\mathbf{p})]_i$, K being the normalization constant. The spin of the photon ceases to be definite and assumes the probability distribution detailed in Figure 5.

The Heisenberg uncertainty products $\Delta X_j \Delta P_j$ along directions parallel and perpendicular to \mathbf{p}_0 are shown in figures (3) and (4); for $s = \pm 1$, both appear monotonically increasing functions of a , converging to $\frac{\hbar}{2}$ in the $a \rightarrow 0$ limit, whereas for $s = 0$ both appear monotonically decreasing functions of a , converging to 1 in the $a \rightarrow 0$ limit. In the opposite limit $a \rightarrow \infty$, the Heisenberg

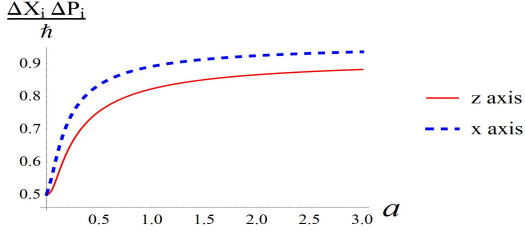


Figure 3. (color online): Heisenberg uncertainty products $\Delta X_j \Delta P_j$ in units of \hbar , along directions parallel (red line) and perpendicular (blue line) to \mathbf{p}_0 , for eigenstates e_s of S_z states with $s = \pm 1$.

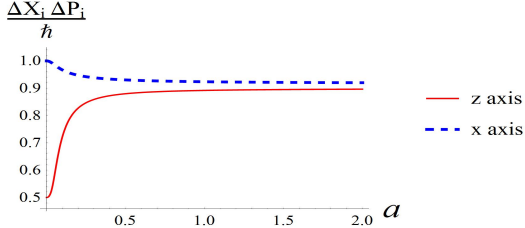


Figure 4. (color online): Heisenberg uncertainty products $\Delta X_j \Delta P_j$ in units of \hbar , along directions parallel (red solid line) and perpendicular (blue dashed line) to \mathbf{p}_0 , for eigenstates e_s of S_z states with $s = 0$.

products converge to finite values detailed in the Supplemental Material. The apparently anomalous behaviour

of the Heisenberg product in figure 4 is a consequence of the fact that the state (24) has, for decreasing a , vanishing projection on the physically relevant subspace \mathcal{H}_S .

V. CONCLUSIONS

In the present work, we have introduced a single-photon state formalism which, only on the basis of simple requirements of special relativity and quantum mechanics, leads to the suppression of the 0-helicity component of the wavefunction. Moreover we have shown how this operation can be interpreted as the action of a projection operator from an auxiliary Hilbert space onto the physical Hilbert space. We have then discussed how this theoretical construction naturally brings along the notion of POVM, and observed how any other observable, in particular the delicate position operator, can be easily introduced as a PVM on the ancillary Hilbert space \mathcal{H}_A and then turned, by means of the projection, into a directly manageable POVMs on \mathcal{H}_S . To illustrate this procedure we have considered the fundamental single-photon observables and have discussed the position-momentum Heisenberg uncertainty relations. In addition we were able to introduce in a very natural way the concept of photon spin in terms of a POVM on \mathcal{H}_S ; in particular, the projection of the spin along the momentum, which represents the helicity operator, has turned out to be a PVM whose eigenvectors correspond to photon states with circular polarization $\left(\frac{\tilde{\psi}_V(p)}{\sqrt{2}}, \frac{\pm i \tilde{\psi}_V(p)}{\sqrt{2}}\right)$.

Moreover, we have extensively investigated the effects of the projection π on gaussian states, which in non-relativistic framework saturate the inequality $\Delta X \Delta P = \frac{\hbar}{2}$. Remarkably, the uncertainty exhibits a non-trivial dependence on the width a of the momentum probability distribution: for any $a > 0$, even in the limit $a \rightarrow \infty$, it remains a finite quantity greater than $\frac{\hbar}{2}$, while for $a \rightarrow 0$ it approaches the minimum value. Such behaviour is observed both for states with definite polarization and spin, confirming the coherence of the underlying formalism, which can be immediately applied to all single-photon states and observables.

Among the possible outlooks we mention the study of angular momentum, the continuous measurement of photon position^{22,23} and propagation of photons, which will form the subject of forthcoming papers. There exist favourable prospects for this formalism to be applied in a high-precision description of interference phenomena at the basis of experiments with single photons^{24–27}.

ACKNOWLEDGEMENTS

The Authors would like to express their deep gratitude to Dr. Andrea Smirne for support and fruitful discussions in merit, and to Dr. Davide Galli, Dr. Ettore Vitali and Prof. Luca Molinari for their useful feedback.

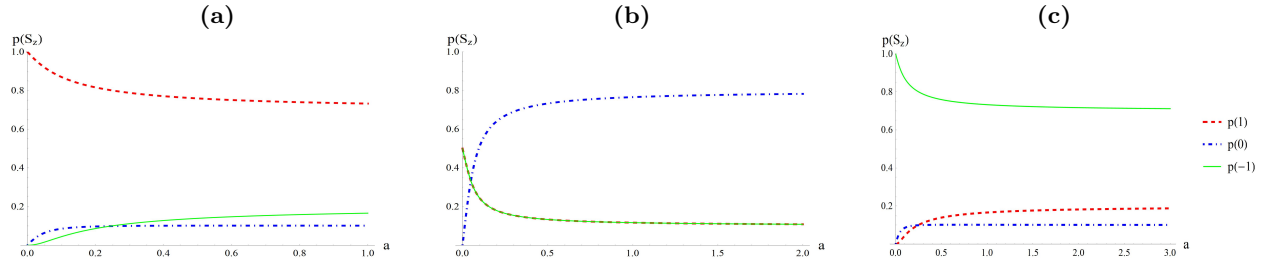


Figure 5. Color online: probability distribution of S_z (red dashed line for the eigenvalue $s = 1$, green solid line for $s = 0$, blue dot-dashed line for $s = -1$) on the spin states (24) with $i=1$ (a), 2 (b), 3 (c)

- ¹ I. Bialynicki-Birula, Phys. Rev. Lett. **80**, 24 (1998)
- ² R. Y. Chiao and Y.-S. Wu, Phys. Rev. Lett. **57**, 933 (1986)
- ³ A. Tomita and R. Y. Chiao, Phys. Rev. Lett. **57**, 937 (1986)
- ⁴ J. E. Sipe, Phys. Rev. A, **52**, 3 (1995)
- ⁵ D. G. Grier, A revolution in optical manipulation, Nature **424**, 810-816 (2003).
- ⁶ K. Kraus, States, Effects and Operations: Fundamental Notions of Quantum Theory, Springer, Berlin (1983).
- ⁷ L.D. Landau, E.M. Lifschitz and L.P. Pitaevskij, Quantum Electrodynamics, Pergamon 2nd Edition (1982)
- ⁸ W.O. Amrein "Localizability of Particles of Mass Zero", Helv. Phys. Acta 42 (1969)
- ⁹ W. Pauli, General Principles of Quantum Mechanics Springer-Verlag, New York, 1980! [translation of Prinzipien der Quantentheorie, Handbuch der Physik Vol. 24 Springer, Berlin, 1933]
- ¹⁰ I. Bialynicki-Birula, in *Progress in Optics*, edited by E. Wolf (Elsevier, Amsterdam, 1996), Vol. XXXVI.
- ¹¹ E. P. Wigner, Ann. Math. **40**, 149 (1939)
- ¹² A.J.Jadzyk, B. Jancewicz "Maximal Localizability of the Photon" Bull.Acad. Pol. Sci. Ser. Math. 21 (1973)
- ¹³ M. Hawton, Phys, Rev, A **59**, 2 (1999)
- ¹⁴ K. Krauss "Position Observable for the Photon" in "Uncertainty Principles and the Foundation of Quantum Mechanics" W.C. Price, S.S: Chissich ed Wiley (1977)
- ¹⁵ A. Peres, Found. Phys. **12**, 1441 (1990)
- ¹⁶ S. Weinberg, The Quantum Theory of Fields, Cap. (2.5) and (5.9) Cambridge University Press (2000)
- ¹⁷ Considering the particular $s = 1$ unitary and irreducible representation of the spin operators \mathbf{S} on \mathbb{C}^3 and the complexification of \mathbb{R}^3 , one has that the operators \mathbf{S} and $i\hbar\mathbf{A}$, with \mathbf{A} denoting the generators of the rotations in \mathbb{R}^3 , satisfy the same commutation relations. Then, the irreducibility of the $s = 1$ representation implies that there exists a unitary transformation V such that $\mathbf{S} = V(i\hbar\mathbf{A})V^\dagger$.
- ¹⁸ M. Hamermesh, Group theory and its application to physical problems, Dover Publications (1989).
- ¹⁹ The term pseudo-Hilbert is inherited from the usual terminology which refers to the pseudo-Riemannian character of the relativistic four-dimensional metric
- ²⁰ T.D. Newton and E.P. Wigner, *Rev. Mod. Phys.* **21**, 400 (1949)
- ²¹ This fact can immediately be checked if we consider that $V\tilde{e}_3(p)$ is the eigenstate of helicity operator $\mathbf{S} \cdot \frac{\mathbf{p}}{|\mathbf{p}|}$ relative to zero eigenvalue.
- ²² A. Barchielli, L. Lanz, G. M. Prosperi, Nuovo Cimento **72B**, 79-121 (1982)
- ²³ A. Holevo, Statistical structure of quantum theory, (Lecture Notes in Physics Monographs) Springer (2001)
- ²⁴ G. Vallone, V. D'Ambrosio, A. Sponselli, S. Slussarenko, L. Marrucci, F. Sciarrino, P. Villoresi, arXiv:1402.2932v1.
- ²⁵ G.S. Paraoanu, Phys. Rev. Lett. **97**, 18 (2006)
- ²⁶ M. Larqué, A. Beveratos, I. Robert-Philip, Eur. Phys. J. D **47**, 119125 (2008)
- ²⁷ A. Beveratos, R. Brouri, T. Gacoin, A. Villing, J.-P. Poizat, P. Grangier, Phys. Rev. Lett. **89**, 187901

Appendix A: Single Photon Formalism

The aim of this appendix is to give further details about the formalism outlined in II.

1. The massless condition

As mentioned in Section II the massless condition naturally pinpoints the subspace $\mathcal{S} \subset \mathcal{H} = \mathcal{L}^2(\mathbb{R}^3, \frac{d^3p}{p^0}) \otimes \mathbb{C}^4$ of elements whose form is most easily specified through the introduction of the *intrinsic frame*. The latter is obtained by transforming the spatial part of the canonical basis $\{e_\mu\}_{\mu=0}^3$ of the Minkowski space through a rotation $R(\mathbf{p})$ of angle $\cos(\phi) = \frac{\mathbf{p}}{|\mathbf{p}|} \cdot \mathbf{e}_3$ around the axis:

$$\mathbf{n} = \frac{\mathbf{e}_3 \wedge \mathbf{p}}{|\mathbf{e}_3 \wedge \mathbf{p}|} \quad (\text{A1})$$

The intrinsic frame is then explicitly given by $\tilde{\mathbf{e}}_i(\mathbf{p}) = R(\mathbf{p}) \mathbf{e}_i$, so that $\tilde{\mathbf{e}}_3(\mathbf{p}) = \frac{\mathbf{p}}{|\mathbf{p}|}$ and:

$$\begin{aligned} \tilde{\mathbf{e}}_1(\mathbf{p}) &= \frac{1}{|\mathbf{p}|} \begin{pmatrix} p_z \\ 0 \\ -p_x \end{pmatrix} + \frac{1}{|\mathbf{p}|^2 \left(1 + \frac{p_z}{|\mathbf{p}|}\right)} \begin{pmatrix} p_y^2 \\ -p_x p_y \\ 0 \end{pmatrix} \\ \tilde{\mathbf{e}}_2(\mathbf{p}) &= \frac{1}{|\mathbf{p}|} \begin{pmatrix} 0 \\ p_z \\ -p_y \end{pmatrix} + \frac{1}{|\mathbf{p}|^2 \left(1 + \frac{p_z}{|\mathbf{p}|}\right)} \begin{pmatrix} p_x p_y \\ p_x^2 \\ 0 \end{pmatrix} \end{aligned} \quad (\text{A2})$$

In light of such change of basis, it can be easily proven that:

$$|\psi_V\rangle \in \mathcal{S} \iff \tilde{\psi}_V^0(\mathbf{p}) = \tilde{\psi}_V^3(\mathbf{p}) \quad (\text{A3})$$

Moreover, for all states $|\psi_V\rangle, |\phi_V\rangle \in \mathcal{S}$:

$$\langle \psi_V | \phi_V \rangle = - \int \frac{d^3p}{p^0} (\psi_V^\mu)^*(p) g_{\mu\nu} \phi_V^\nu(p) = \sum_{i=1,2} \int \frac{d^3p}{p^0} (\tilde{\psi}_V^i)^*(p) \tilde{\phi}_V^i(p) \quad (\text{A4})$$

Equation (A4) clearly implies that the restriction of the inner product (7) to \mathcal{S} is non-negative and does not depend on the components $\tilde{\psi}_V^0 = \tilde{\psi}_V^3$ and $\tilde{\phi}_V^0 = \tilde{\phi}_V^3$.

Since \mathcal{S} contains non-zero elements with vanishing norm, it is not a proper Hilbert space. Nevertheless, one can introduce a Hilbert space from \mathcal{S} by observing that

$$|\psi_V\rangle \sim |\phi_V\rangle \quad \text{if } \tilde{\psi}_V^1(\mathbf{p}) = \tilde{\phi}_V^1(\mathbf{p}) \text{ and } \tilde{\psi}_V^2(\mathbf{p}) = \tilde{\phi}_V^2(\mathbf{p}) \quad (\text{A5})$$

is an equivalence relation on \mathcal{S} , and therefore the quotient \mathcal{S}/\sim is a Hilbert space with null vector:

$$[0] = \{|\psi_V\rangle \in \mathcal{S} : \tilde{\psi}_V^1(\mathbf{p}) = 0, \tilde{\psi}_V^2(\mathbf{p}) = 0\} \quad (\text{A6})$$

We remark that the mathematical structure of the pseudo-Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathbb{R}^3, \frac{d^3p}{p^0}) \otimes \mathbb{C}^4$ plays a crucial role when the Fock space is constructed in order to describe many-photons systems. The field theory obtained in this framework is consistent with Gupta and Bleuler's formulation (S. Gupta, *Proc. Phys. Soc.* **A63**, 681 (1950) ; K. Bleuler, *Helv. Phys. Acta* **23**, 567 (1950)), as it will be shown in a forthcoming paper.

Appendix B: The Newton-Wigner Position Operator

In this Appendix we will present the theory of localization of the single photon following the historical construction by Newton and Wigner, which introduced the concept for massive and spinless particles. This will form the basis for the case at hand of massless and spin $s = 1$ particles, for which we will specify in this Appendix the transformation properties of the operator.

1. The Newton-Wigner Operator for massive particles

The description of a spin $s = 0$ relativistic particle is notoriously set in the Hilbert space $L^2\left(\mathbb{R}^3, \frac{d^3p}{p^0}\right)$, related to $L^2(\mathbb{R}^3, d^3p)$ by the isometric isomorphism

$$\psi(\mathbf{p}) \in L^2(\mathbb{R}^3, d^3p) \mapsto \sqrt{p^0} \psi(\mathbf{p}) \in L^2\left(\mathbb{R}^3, \frac{d^3p}{p^0}\right) \quad (\text{B1})$$

Correspondingly starting with the generalized eigenfunction of $\hat{X} = i\hbar \frac{\partial}{\partial \mathbf{p}}$ in $L^2(\mathbb{R}^3, d^3p)$

$$\langle \mathbf{p} | \mathbf{x} \rangle = \frac{e^{-\frac{i}{\hbar} \mathbf{x} \cdot \mathbf{p}}}{(2\pi\hbar)^{\frac{3}{2}}} \quad (\text{B2})$$

with eigenvalue \mathbf{x} , we have the generalized eigenfunction for the relativistic case

$$\sqrt{p^0} \frac{e^{-\frac{i}{\hbar} \mathbf{x} \cdot \mathbf{p}}}{(2\pi\hbar)^{\frac{3}{2}}} \quad (\text{B3})$$

which, as a simple calculation shows, are in turn generalized eigenfunctions of the Newton-Wigner position operator $\hat{X}_{NW} = i\hbar \frac{\partial}{\partial \mathbf{p}} - \frac{i\hbar}{2} \frac{\mathbf{p}}{(p^0)^2}$ with eigenvalue \mathbf{x} .

2. Transformation Properties of the Newton-Wigner Operator

As long as massive spinless particles are considered, it can be easily shown that the Newton-Wigner position operator is covariant under roto-translations. In fact, since $L^2\left(\mathbb{R}^3; \frac{d^3p}{p^0}\right)$ carries the following irreducible representation of the Poincaré group:

$$U(a, \Lambda)\psi(p) = e^{-\frac{i}{\hbar} a_\mu p^\mu} \psi(\Lambda^{-1}p) \quad (\text{B4})$$

which for a roto-translation particularizes to:

$$U(\mathbf{a}, R)\psi(p) = e^{-\frac{i}{\hbar} \mathbf{a} \cdot \mathbf{p}} \psi(R^{-1}\mathbf{p}) \quad (\text{B5})$$

yielding:

$$U^\dagger(\mathbf{a}, R) \hat{X}_{NW} U(\mathbf{a}, R) = R \hat{X}_{NW} + \mathbf{a} \hat{I} \quad (\text{B6})$$

Equation (B6) ensures that the the Newton-Wigner position is covariant under roto-translation, a necessary requirement for any localization observable. On the contrary, for a boost Λ of velocity $\boldsymbol{\beta}$ one has:

$$U(0, \Lambda) |\mathbf{x}\rangle = U(a, \mathbb{I}) \left| \mathbf{x} + \frac{\gamma - 1}{\beta^2} \boldsymbol{\beta} \cdot \mathbf{x} \boldsymbol{\beta} \right\rangle \quad (\text{B7})$$

with $a = (\gamma \boldsymbol{\beta} \cdot \mathbf{x}, 0)$: the right member of equation (B7) is the image of an eigenstate of position through a time displacement operator $U(a, \mathbb{I})$, rather than an eigenstate of position itself, so that the Newton-Wigner POVM is not covariant under boosts. This circumstance is expected, due to the fact that, in a measuring process of position, a particle is localized in a space region \mathcal{M} at a time instant t , and the space-time region $\{t\} \times \mathcal{M}$ is obviously not preserved under boosts.

3. Position Statistics

From equation (18), by taking the marginal over the spin degrees of freedom, we are left with the following position probability distribution:

$$p(\mathbf{X} \in \mathcal{M}, S_z = s) = \int_{\mathcal{M}} d^3x \sum_{s=1}^3 \left| \left[\tilde{\psi}_V(\mathbf{x}) \right]_s \right|^2 \quad (\text{B8})$$

Inserting in (B8) the definition (19) of $\left[\tilde{\psi}_V(\mathbf{x})\right]_s$, we readily find that the first momenta of (B8) are given by:

$$\begin{aligned}\langle X_k \rangle &= i\hbar \sum_{s=1}^3 \int d^3p \left[\tilde{\phi}_V^*(p)\right]_s \frac{\partial}{\partial p_k} \left[\tilde{\phi}_V(p)\right]_s \\ \langle X_k^2 \rangle &= -\hbar^2 \sum_{s=1}^3 \int d^3p \left[\tilde{\phi}_V^*(p)\right]_s \frac{\partial^2}{\partial p_k^2} \left[\tilde{\phi}_V(p)\right]_s\end{aligned}\tag{B9}$$

where

$$\left[\tilde{\phi}_V(p)\right]_s = \frac{\left[\tilde{\psi}_V(p)\right]_s}{\sqrt{|\mathbf{p}|}} = \frac{1}{\sqrt{|\mathbf{p}|}} \sum_{i=1}^2 \tilde{\psi}_V^i(p) [V\tilde{e}_i(p)]_s\tag{B10}$$

Appendix C: Calculation Details

The aim of this appendix is to describe in detail the computational procedure which led to the results shown in figures 2, 3, 4 and 5.

1. States with Definite Polarization

For states in \mathcal{H}_S of the form (22) the square norm is obtained from a straightforward calculation:

$$\langle \tilde{\psi}_V(\mathbf{p}) | \tilde{\psi}_V(\mathbf{p}) \rangle = \sum_{k=1}^2 |\gamma_k|^2\tag{C1}$$

so that, if $\sum_{k=1}^2 |\gamma_k|^2 = 1$, the mean value and the variance of momentum are given by:

$$\begin{aligned}\langle P^j \rangle &= p_0^j \\ \langle (P^j)^2 \rangle &= (p_0^j)^2 + 2a(p_0^j)^2\end{aligned}\tag{C2}$$

On the contrary, the calculation of the expectation and variance of position is complicated by the circumstance that the gradient appearing in (B9) acts non-trivially on the vectors $e_k(\mathbf{p})$. Applying formula (B9) to the states (22), one finds that the mean values of X_j and X_j^2 are bilinear functions of the coefficients γ_j , described by the matrices

$$\begin{aligned}[\mathbf{X}^j]_{kl} &= i\hbar \int d^3p \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{4ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{2}}} e_k(\mathbf{p}) \cdot \partial_{\mathbf{p}_j} e_l(\mathbf{p}) + \mathbf{x}_0^j \delta_{kl} \\ [(\mathbf{X}^j)^2]_{kl} &= -\hbar^2 \int d^3p \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{4ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{2}}} \left[e_k(\mathbf{p}) \cdot \partial_{\mathbf{p}_j}^2 e_l(\mathbf{p}) - \frac{p_j - p_{0j}}{4ap_0^2} e_k(\mathbf{p}) \cdot \partial_{\mathbf{p}_j} e_l(\mathbf{p}) \right] + \delta_{kl} \frac{\hbar^2}{8ap_0^2} + (x_0^j)^2 \delta_{kl}\end{aligned}\tag{C3}$$

Performing the integrations (C3) one finds:

$$\begin{aligned}[X_j]_{kl} &= 0 \quad \forall j = 1, 2, 3 \\ [(X^3)^2]_{kl} &\equiv [(Z)^2]_{kl} = \delta_{kl} \frac{1 - 4a + 4\sqrt{a}(1 + 2a) \mathcal{D}\left(\frac{1}{2\sqrt{a}}\right)}{8ap_0^2} \\ [(X^1)^2]_{kl} &\equiv [(X)^2]_{kl} = \delta_{kl} u(a) \\ [(X^2)^2]_{kl} &\equiv [(Y)^2]_{kl} = \delta_{kl} u(a)\end{aligned}\tag{C4}$$

where $\mathcal{D}(x)$ is the Dawson's function (sometimes also referred to as Dawson's Integral) of argument x (for details about properties see e.g. M. Abramowitz, I. Stegun *Handbook of Mathematical Functions* (1964)).

To the best of our knowledge, no analytic expression can be given for the function $u(a)$. Its behaviour for small a can be captured substituting the function which multiplies the gaussian measure in (C3) with its expansion around p_0 :

$$-\frac{1}{8ap_0^2} + \frac{1}{p_0^2} + \frac{p_x^2}{16a^2p_0^4} - \frac{2(p_0 - p_z)}{p_0^3} - \frac{8p_x^2 + 3p_y^2 - 12(p_z - p_0)^2}{4p_0^4} \quad (\text{C5})$$

Under this approximation one gets:

$$u(a) \simeq \frac{1 + 8a + 4a^2 + 56a^3}{8ap_0^2} \quad (\text{C6})$$

which provides a satisfactory approximation up to $a \simeq 0.01$.

To compute $\Delta X \Delta P_x$ for all values of a , we performed a numerical integration of (C3), obtaining the estimates listed in table C 1. We fitted them to the ansatz:

$$f(x) = \alpha_1 + \alpha_2 e^{-\alpha_3 x} + \alpha_4 e^{-\alpha_5 x} \quad (\text{C7})$$

and represented the latter in figure 2.

a	$\frac{\Delta X \Delta P_x}{h}$
0.000	0.5000
0.001	0.5020
0.002	0.5040
0.005	0.5099
0.01	0.5197
0.02	0.5390
0.05	0.5960
0.1	0.6756
0.2	0.7650
0.5	0.8679
1	0.9462
1.1	0.9578
1.5	0.9978
2.0	0.9997

Table I. numeric estimates of the function $\frac{\Delta X \Delta P_x}{h}$, with precision 10^{-4} .

2. Spin States

For states in $\overline{\mathcal{H}}_{\mathcal{A}}$ of the form

$$\mathbf{f}(\mathbf{p}) = \sqrt{|\mathbf{p}|} \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{8ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{4}}} \mathbf{h} \quad (\text{C8})$$

which particularizes (24) when $\mathbf{h} = \mathbf{e}_i$, the corresponding physical states on $\mathcal{H}_{\mathcal{S}}$ are given by

$$\tilde{\psi}_V(\mathbf{p}) = \mathbf{K} (\mathbf{V}\pi\mathbf{V}^\dagger \mathbf{f}) (\mathbf{p}) \quad (\text{C9})$$

with $\mathbf{K}^{-1} = \langle \tilde{\psi}_V(\mathbf{p}) | \tilde{\psi}_V(\mathbf{p}) \rangle$ being the normalization constant. Straightforward calculations show that \mathbf{K} and the first momenta of $\hat{\mathbf{P}}$ and $\hat{\mathbf{X}}$ are quadratic functions of \mathbf{h} , and thus are described by the following matrices:

$$\mathbf{K} = \int d^3p \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{4ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{2}}} \mathbf{\Pi}(\mathbf{p}) \quad (\text{C10})$$

$$\mathbf{P}_j = \int d^3p \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{4ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{2}}} p_j \mathbf{\Pi}(\mathbf{p}) \quad (\text{C11})$$

$$\mathbf{P}^2_j = \int d^3p \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{4ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{2}}} p_j^2 \mathbf{\Pi}(\mathbf{p}) \quad (\text{C12})$$

$$\mathbf{X}_j = i\hbar \int d^3p \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{4ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{2}}} \left[\frac{\partial}{\partial p_j} \mathbf{\Pi}(\mathbf{p}) - \frac{p_j - p_{0j}}{4ap_0^2} \mathbf{\Pi}(\mathbf{p}) \right] \quad (\text{C13})$$

$$\mathbf{X}^2_j = -\hbar^2 \int d^3p \frac{e^{-\frac{|\mathbf{p}-\mathbf{p}_0|^2}{4ap_0^2}}}{(4\pi ap_0^2)^{\frac{3}{2}}} \left[\frac{\partial^2}{\partial p_j^2} \mathbf{\Pi}(\mathbf{p}) - 2 \frac{p_j - p_{0j}}{4ap_0^2} \frac{\partial}{\partial p_j} \mathbf{\Pi}(\mathbf{p}) + \left[\left(\frac{p_j - p_{0j}}{4ap_0^2} \right)^2 - \frac{1}{4ap_0^2} \right] \mathbf{\Pi}(\mathbf{p}) \right] \quad (\text{C14})$$

where we have called $\mathbf{\Pi}(\mathbf{p}) = \mathbf{V}\pi\mathbf{V}^\dagger$, making explicit its dependence on \mathbf{p} (which is not anymore trivial as in π because of the action of the matrix \mathbf{V}). We list below their analytic expression, resulting from a calculations in spherical coordinates. Remarkably, all the results can be expressed in terms of the following two functions:

$$\begin{aligned} u_1(a) &= 1 - 6a + 12a^{3/2} \mathcal{D} \left(\frac{1}{2\sqrt{a}} \right) \\ u_2(a) &= 1 - 2\sqrt{a} \mathcal{D} \left(\frac{1}{2\sqrt{a}} \right) \end{aligned} \quad (\text{C15})$$

$\mathcal{D}(x)$ denoting the Dawson's integral.

$$\mathbf{K} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + 2a u_2(a) \begin{pmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (\text{C16})$$

$$\mathbf{P}^1 \equiv \mathbf{P}_x = 2p_0 a u_1(a) \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \quad (\text{C17})$$

$$\mathbf{P}^2 \equiv \mathbf{P}_y = 2p_0 a u_1(a) \begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} \\ 0 & -\frac{i}{\sqrt{2}} & 0 \end{pmatrix} \quad (\text{C18})$$

$$\mathbf{P}^3 \equiv \mathbf{P}_z = p_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + 2p_0 a u_1(a) \begin{pmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (\text{C19})$$

$$(\mathbf{P}^1)^2 = (2p_0)^2 \frac{a}{2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (2p_0)^2 a^2 u_1(a) \begin{pmatrix} -2 & 0 & 1 \\ 0 & 4 & 0 \\ 1 & 0 & -2 \end{pmatrix} \quad (\text{C20})$$

$$(\mathbf{P}^2)^2 = (2p_0)^2 \frac{a}{2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (2p_0)^2 a^2 u_1(a) \begin{pmatrix} -2 & 0 & -1 \\ 0 & 4 & 0 \\ -1 & 0 & -2 \end{pmatrix} \quad (\text{C21})$$

$$(\mathbf{P}^3)^2 = p_0^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 4a & 0 \\ 0 & 0 & 1 \end{pmatrix} + (2p_0)^2 4a^2 u_1(a) \begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (\text{C22})$$

$$\mathbf{X}^3 \equiv \mathbf{Z} = 0 \quad (\text{C23})$$

$$\mathbf{X}^1 \equiv \mathbf{X} = 0$$

$$\mathbf{X}^2 \equiv \mathbf{Y} = 0$$

$$\begin{aligned} (\mathbf{X}^1)^2 &= \frac{\hbar^2}{p_0^2} \begin{pmatrix} \frac{1}{2}u_1(a) - u_2(a)\left(\frac{1}{2} + \frac{1}{4a}\right) + \frac{3}{8a} & 0 & -\frac{u_1(a)+2u_2(a)}{4} \\ 0 & 2u_2(a) - u_1(a) & 0 \\ -\frac{u_1(a)+2u_2(a)}{4} & 0 & \frac{1}{2}u_1(a) - u_2(a)\left(\frac{1}{2} + \frac{1}{4a}\right) + \frac{3}{8a} \end{pmatrix} \\ (\mathbf{X}^2)^2 &= \frac{\hbar^2}{p_0^2} \begin{pmatrix} \frac{1}{2}u_1(a) - u_2(a)\left(\frac{1}{2} + \frac{1}{4a}\right) + \frac{3}{8a} & 0 & \frac{u_1(a)+2u_2(a)}{4} \\ 0 & 2u_2(a) - u_1(a) & 0 \\ \frac{u_1(a)+2u_2(a)}{4} & 0 & \frac{1}{2}u_1(a) - u_2(a)\left(\frac{1}{2} + \frac{1}{4a}\right) + \frac{3}{8a} \end{pmatrix} \\ (\mathbf{X}^3)^2 &= \frac{\hbar^2}{p_0^2} \begin{pmatrix} \frac{1}{4a} + \frac{4a-1}{8a}u_2(a) - u_1(a) & 0 & 0 \\ 0 & \frac{3}{4a} - \frac{12a+3}{4a}u_2(a) + 2u_1(a) & 0 \\ 0 & 0 & \frac{1}{4a} + \frac{4a-1}{8a}u_2(a) - u_1(a) \end{pmatrix} \end{aligned} \quad (\text{C24})$$

The matrices associated to the components of momentum and position observable along the x and y axes differ one from each other, but share the same spectrum. The results presented in figures (3) and (4) are readily obtained from equations (C16) and (C23), once \hbar is put equal to $\hbar = (1, 0, 0)$, and to $(0, 1, 0)$. In such cases, the Heisenberg

uncertainty products on the z and x axis, respectively parallel and perpendicular to \mathbf{p}_0 , read:

$$\begin{aligned}
\frac{\Delta Z \cdot \Delta P_z}{\hbar} &= \frac{\sqrt{\left[1 + 16a^2 u_1(a) - \frac{(1-2a u_1(a))^2}{1-2a u_2(a)}\right] \left[\frac{1}{4a} + \left(\frac{1}{2} - \frac{1}{8a}\right) u_2(a) - u_1(a)\right]}}{1 - 2a u_2(a)} \\
\frac{\Delta X \cdot \Delta P_x}{\hbar} &= \frac{\sqrt{2a(1 - 4a u_2(a)) \left(\frac{1}{2} u_1(a) - u_2(a) \left(\frac{1}{2} + \frac{1}{4a}\right) + \frac{3}{8a}\right)}}{1 - 2a u_2(a)} \\
\frac{\Delta Z \cdot \Delta P_z}{\hbar} &= \frac{\sqrt{\frac{1}{a} [(1 - 8a u_1(a)) u_2(a) - u_1^2(a)] \left(\frac{3}{4a} - \left(3 + \frac{3}{4a}\right) u_2(a) + 2u_1(a)\right)}}{2u_2(a)} \\
\frac{\Delta X \cdot \Delta P_x}{\hbar} &= \frac{\sqrt{u_1(a) (2u_2(a) - u_1(a))}}{u_2(a)}
\end{aligned} \tag{C25}$$

We conclude this section considering a generic $\mathbf{h} \in \mathbb{C}^3$ that, for the purpose of simplifying the forthcoming calculations, will be parametrized as follows:

$$\mathbf{h} = \begin{pmatrix} \frac{\tilde{h}_1}{\sqrt{1-2au(a)}} \\ \frac{\tilde{h}_2}{\sqrt{4au(a)}} \\ \frac{\tilde{h}_3}{\sqrt{1-2au(a)}} \end{pmatrix} \tag{C26}$$

assuming, without loss of generality, $|\tilde{h}_1|^2 + |\tilde{h}_2|^2 + |\tilde{h}_3|^2 = 1$. This choice leads to the following expressions:

$$\begin{aligned}
\langle P_z \rangle &= p_0 \left[\frac{1 - 2au_1(a)}{1 - 2au_2(a)} (1 - \rho) + \frac{u_1(a)}{u_2(a)} \rho \right] \\
\langle (P_z)^2 \rangle &= p_0^2 \left[\frac{1 + 16a^2 u_1(a)}{1 - 2au_2(a)} (1 - \rho) + \frac{1 - 8au_1(a)}{u_2(a)} \rho \right] \\
\langle Z \rangle &= 0 \\
\langle Z^2 \rangle &= \frac{\hbar^2}{p_0^2} \left[\frac{\frac{1}{4a} + \frac{u_2(a)}{2} + \frac{u_2(a)}{8a} - u_1(a)}{1 - 2au_2(a)} (1 - \rho) + \frac{\frac{3}{4a} - \left(3 + \frac{3}{4a}\right) u_2(a) + 2u_1(a)}{4au_2(a)} \rho \right]
\end{aligned} \tag{C27}$$

where $|\tilde{h}_2|^2 = \rho$, $|\tilde{h}_1|^2 + |\tilde{h}_3|^2 = 1 - \rho$. The square of the Heisenberg product constructed from (C27) is a polynomial of third degree in the variable ρ possessing, for each fixed value of a , a global maximum at a value $\rho_{max}(a)$ in the interval $(0, 1)$ and a global minimum at $\rho_{min}(a) = \Theta(a - a^*)$, where $a^* \sim 6.13116$. We do not detail the rather intricate analytic form of the minimum and maximum values of the Heisenberg product, but limit ourselves to show, in figure 6, their values against those 3 and (4) relative to the choices $\mathbf{h} = (1, 0, 0)$ and $\mathbf{h} = (0, 1, 0)$.

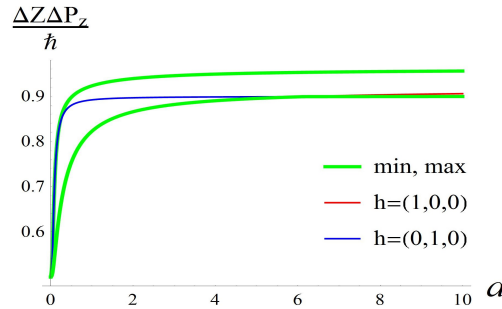


Figure 6. (color online) minimum and maximum (green lines) of the Heisenberg uncertainty product along the z axis, in comparison with $\mathbf{h} = (0, 0, 1)$ (red line) and $\mathbf{h} = (0, 1, 0)$ (blue line).

On the x axis, it is convenient to parametrize also \tilde{h} as follows:

$$\tilde{\mathbf{h}} = \begin{pmatrix} \sqrt{\lambda} e^{i\phi_1} \\ \sqrt{1-\lambda}\sqrt{\xi} \\ \sqrt{1-\lambda}\sqrt{1-\xi} e^{i\phi_2} \end{pmatrix} \quad (\text{C28})$$

obtaining:

$$\begin{aligned} \langle \hat{P}_x \rangle &= -(2p_0) \frac{2au_1(a)}{\sqrt{(1-2au_2(a))(4au_2(a))}} (1-\lambda) \sqrt{\xi-\xi^2} \cos(\phi_2) \\ \langle (\hat{P}_x)^2 \rangle &= (2p_0)^2 a \left[\frac{1-2au_1(a)}{2(1-2au_2(a))} \lambda + \frac{1-6au_1(a)}{2(1-2au_2(a))} (1-\lambda)(1-\xi) + \frac{u_1(a)}{u_2(a)} (1-\lambda)\xi \right] \\ \langle \hat{X} \rangle &= 0 \\ \langle \hat{X}^2 \rangle &= \frac{\hbar^2}{(2p_0)^2} \left[\frac{u_1(a) - \frac{u_2(a)}{a} - 4u_2(a) + \frac{3}{2a}}{1-2au_2(a)} \lambda + \right. \\ &\quad \left. + \frac{3u_1(a) - u_2(a) + \frac{3}{2a}}{1-2au_2(a)} (1-\lambda)(1-\xi) + \frac{2u_2(a) - u_1(a)}{au_2(a)} (1-\lambda)\xi \right] \end{aligned}$$

The square of the Heisenberg uncertainty product is a linear and monotonically decreasing function of $\cos^2(\phi_2)$. The minimum is attained at $\cos^2(\phi_2) = 1$, $\xi = 0$ and $\lambda = \Theta(a^* - a)$, $a^* \sim 2.6095$, and the maximum at $\cos^2(\phi_2) = 0$, $\xi = \xi_{max}(a)$ and $\lambda = 0$. $\xi_{max}(a)$ results from a straightforward but quite lengthy maximization procedure. The minimum and maximum values of the Heisenberg uncertainty product are shown in Fig. C 2 against the corresponding values (C25) for $\mathbf{h} = (1, 0, 0)$ and $\mathbf{h} = (0, 1, 0)$.

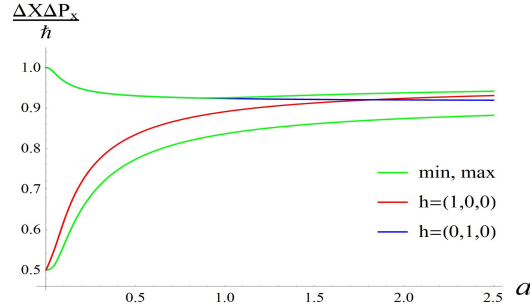


Figure 7. (color online) minimum and maximum (green lines) of the Heisenberg uncertainty product along the x axis, in comparison with $\mathbf{h} = (0, 0, 1)$ (red line) and $\mathbf{h} = (0, 1, 0)$ (blue line).

3. Probability Distribution of S_z

In this section we give the explicit expression for the probability distribution of S_z for a spin state of the form (C8):

$$p(S_z = s) = \frac{\sum_{ij} \mathbf{h}_i^* \Sigma(s)_{ij} \mathbf{h}_j}{\sum_{ij} \mathbf{h}_i^* \mathbf{K}_{ij} \mathbf{h}_j} \quad (\text{C29})$$

where

$$\Sigma(s)_{ij} = \int \frac{d^3 \mathbf{p}}{p^0} \Pi(p)_{si}^* \Pi(p)_{sj} \quad (\text{C30})$$

\mathbf{h}	axis	small a	large a
$(1, 0, 0)$	z	$\frac{1}{2} + 4a^2$	$\frac{\sqrt{21}}{5} - \frac{59\sqrt{3}}{350\sqrt{7}a}$
$(1, 0, 0)$	x	$\frac{1}{2} + a + 40a^3$	$\frac{3\sqrt{41}}{2} - \frac{1381}{2800\sqrt{41}a}$
$(0, 1, 0)$	z	$\frac{1}{2} + 16a^2 + 272a^3$	$\frac{9}{10} - \frac{1}{175a}$
$(0, 1, 0)$	x	$1 - 8a^2 + 32a^3$	$\frac{\sqrt{21}}{5} + \frac{2\sqrt{3}}{175\sqrt{7}a}$
(h_1, h_2, h_3)	z (min)	$\frac{1}{2} + 4a^2$	$\frac{9}{10} - \frac{1}{175a}$
(h_1, h_2, h_3)	z (max)	$\frac{1}{2} + \frac{a}{2} + 12a^2$	$2\sqrt{\frac{3}{13}} - \frac{317}{3640a}\sqrt{\frac{3}{13}}$
(h_1, h_2, h_3)	x (min)	$\frac{1}{2} + 4a^2$	$\frac{9}{10} - \frac{23}{525a}$
(h_1, h_2, h_3)	x (max)	$1 - 8a^2 + 32a^3$	$2\sqrt{\frac{3}{13}} - \frac{1021}{9100}\sqrt{\frac{3}{13}} \frac{1}{a}$

and \mathbf{K} is the normalization constant introduced above. Equation (C29) is then a ratio between two quadratic functions of \mathbf{h} . The denominator is explicitly given by (C16), while the matrix $\mathbf{\Sigma}(\mathbf{s})$ in the numerator reads

$$\begin{aligned}
\mathbf{\Sigma}(\mathbf{1}) &= \begin{pmatrix} 4a + (1 - 6a)(1 - 2au_2(a)) & 0 & 0 \\ 0 & 2(1 + 12a)(1 - 2au_2(a)) - (1 + 8a) & 0 \\ 0 & 0 & 1 + 4a - (1 + 6a)(1 - 2au_2(a)) \end{pmatrix} \\
\mathbf{\Sigma}(\mathbf{0}) &= \begin{pmatrix} 4a - (2a + 24a^2)u_2(a) & 0 & 0 \\ 0 & (1 + 6a)8u_2(a) - 4a & 0 \\ 0 & 0 & 4a - (2a + 24a^2)u_2(a) \end{pmatrix} \\
\mathbf{\Sigma}(-\mathbf{1}) &= \begin{pmatrix} 1 + 4a - (1 + 6a)(1 - 2au_2(a)) & 0 & 0 \\ 0 & 2(1 + 12a)(1 - 2au_2(a)) - (1 + 8a) & 0 \\ 0 & 0 & 4a + (1 - 6a)(1 - 2au_2(a)) \end{pmatrix}
\end{aligned} \tag{C31}$$

from which it is evident that:

- a) $p(S_z = 1) = p(S_z = -1)$ for the spin state relative to the choice $\mathbf{h} = (0, 1, 0)$
- b) $p(S_z = 1)$ for the spin state with $\mathbf{h} = (1, 0, 0)$ and $p(S_z = -1)$ for the spin state with $\mathbf{h} = (0, 0, -1)$ are equal to each other.

The asymptotic behaviour of the probability distributions shown in figure (5) is listed in the following table (C3).

S_z	h	small a	large a
1	(1,0,0)	$1 - 2a + 8a^2$	$\frac{7}{10} + \frac{51}{1400a}$
0	(1,0,0)	$2a - 16a^2$	$\frac{1}{10} + \frac{3}{1400a}$
-1	(1,0,0)	$8a^2$	$\frac{2}{10} - \frac{54}{1400a}$
1	(0,1,0)	$\frac{1}{2} - 4a + 8a^2$	$\frac{1}{10} + \frac{3}{175a}$
0	(0,1,0)	$8a - 16a^2$	$\frac{8}{10} - \frac{6}{175a}$

Table II. asymptotic behaviour of the probability distribution of S_z for the choices of h reported in figure 5.